netlognews

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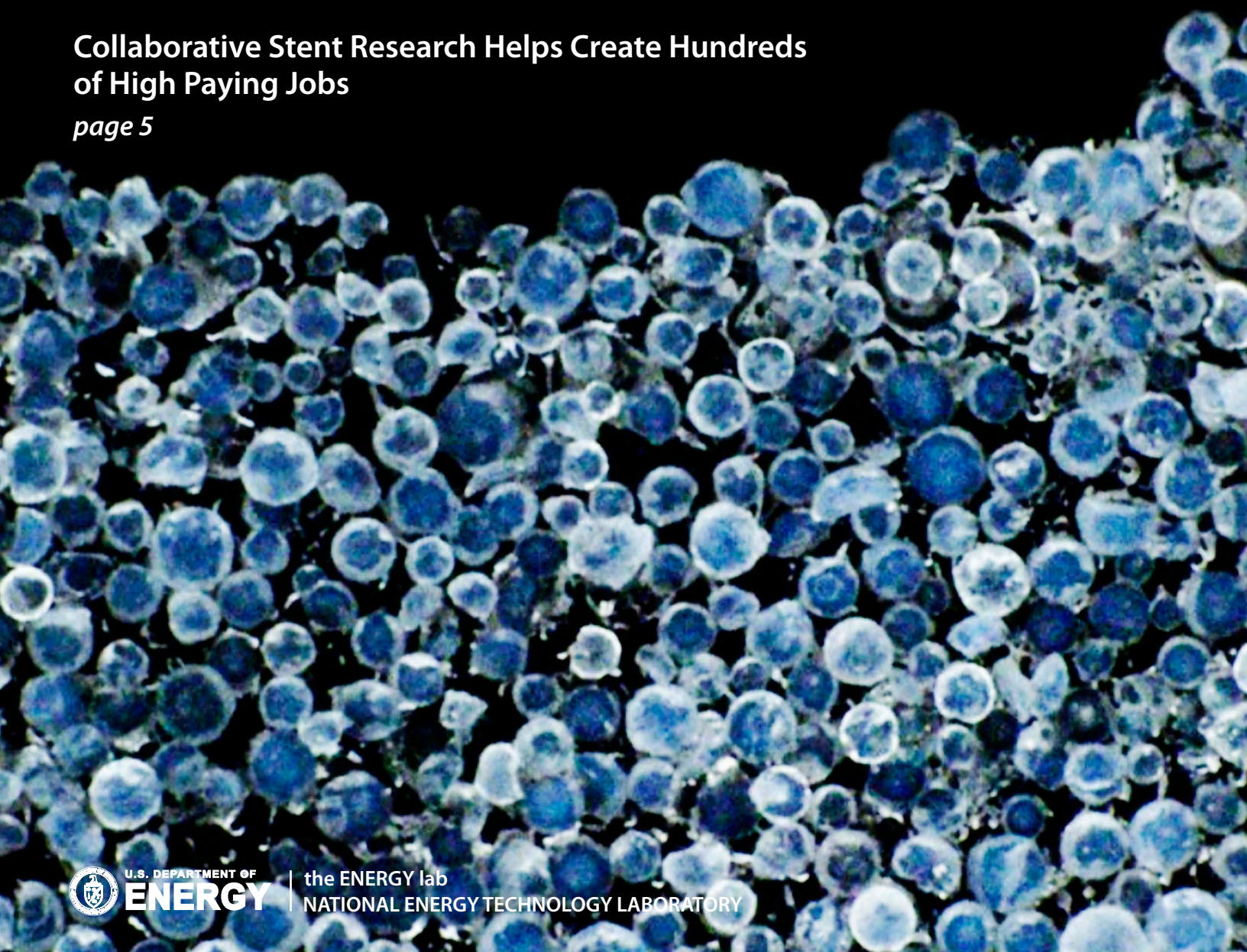

U.S. DEPARTMENT OF ENERGY | the ENERGY lab
NATIONAL ENERGY TECHNOLOGY LABORATORY

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Cover image: NETL-Developed Capture Technology Wins 2012 R&D Award

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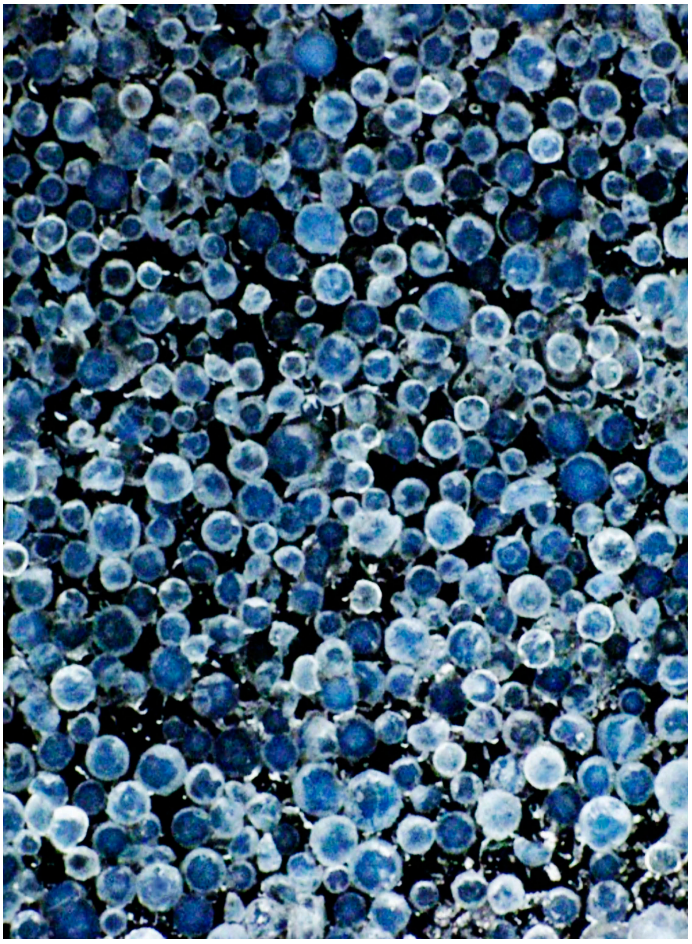
newlognews is a quarterly newsletter that highlights recent achievements and ongoing research at NETL. Any comments or suggestions, please contact Paula Turner at paula.turner@netl.doe.gov or call 541-967-5966.



Sorbent pellets of immobilized polyethylenimine on the support CARiACT Q10, a commercial silica gel support with a diameter of 100 to 350 µm. Sorbent pellets were prepared in two 600-lb batches by Pressure Chemical Company.

NETL-Developed Carbon Capture Technology Wins 2012 R&D 100 Award

—A novel carbon capture technology developed at the National Energy Technology Laboratory has been recognized by *R&D Magazine* as among the 100 most technologically significant products introduced into the commercial marketplace within the past year. This year's award recognizes NETL's patented and patent-pending technologies that capture CO_2 from flue gas streams.

CO_2 is one of the major greenhouse gases impacting climate change, and nearly one-third of man-made CO_2 emissions result from the combustion of fossil fuels for electricity generation. NETL has been investigating ways to control CO_2 emissions from power plants using the two-step carbon sequestration process (carbon capture followed by permanent storage). NETL's "Basic Immobilized Amine Sorbent (BIAS) Process for CO_2 Capture" is one result of this effort. This process advances the capture of CO_2 from power plants, preventing its release into the air. The captured CO_2 can then be permanently stored in a carbon sequestration scenario.

The process encompasses a portfolio of techniques for producing regenerable immobilized amine-based sorbents and provides a method for capturing CO_2 from flue gas streams. Low-cost, regenerable amine-based sorbents offer many advantages over existing technologies including increased CO_2 capture capacity, reduced corrosion, lower energy requirements and costs, and minimized water usage. Additionally, amine-based sorbents are scalable for use in industrial applications, including coal combustion and gasification-based power generating systems.

This technology can be used to reduce cost and energy associated with more conventional scrubbing processes, both as a retrofit to older power plants that currently burn coal or applied to new, more efficient pulverized coal-fired power plants. Additionally, the BIAS process can capture CO_2 from utilities that combust oil or natural gas. Although the process is envisioned for use primarily as a postcombustion CO_2 capture method for power generation point sources, BIAS sorbents are also being considered for other applications, such as natural gas cleanup, life support systems/confined spaces, and air capture systems.

R&D 100 Awards identify state-of-the art technologies and help move innovative science into the public marketplace. Congratulations to McMahan Gray, Henry Pennline, Daniel Fauth, James Hoffman, and Kevin Resnik of the BIAS team for this prestigious recognition.

Water sample being injected into the tested carbonation meter using a 140-mL syringe and an in-line 0.45-µm filter.

Field-proven Meter Rapidly Determines Carbon Dioxide Levels in Groundwater

—NETL and West Virginia University collaborators discovered that a standard beverage industry carbonation meter used with a modified field protocol accurately determined the amount of CO_2 dissolved in natural springs and mine waters within the range of 0.2 - 35 millimole (a mole is a measurement for chemicals, thus a millimole is one thousandth of a mole) of CO_2. The meter, which measures dissolved CO_2 based on temperature and pressure changes determined during sample volume expansion, offers a new way to measure dissolved CO_2 rapidly and reproducibly in a wide range of natural waters, which is critical when investigating possible leakage from carbon sequestration sites. Estimates of dissolved CO_2 concentrations using conventional titration approaches are time-consuming, and results can vary widely because of various sources of error (e.g., rapid degassing, low alkalinity, non-carbonate alkalinity). Carbonation meter measurements compared well with those obtained with more conventional approaches, but were immediate and avoided errors introduced by alkalinity. The portable meter is practical for use in difficult terrain, and the technique proved useful for studying aquatic systems in which CO_2 degassing drives geochemical changes that result in mineral precipitation and deposition. Selected results of this research appear in Elsevier's *Journal of Hydrology* (doi:10.1016/j.jhydrol.2012.03.015).

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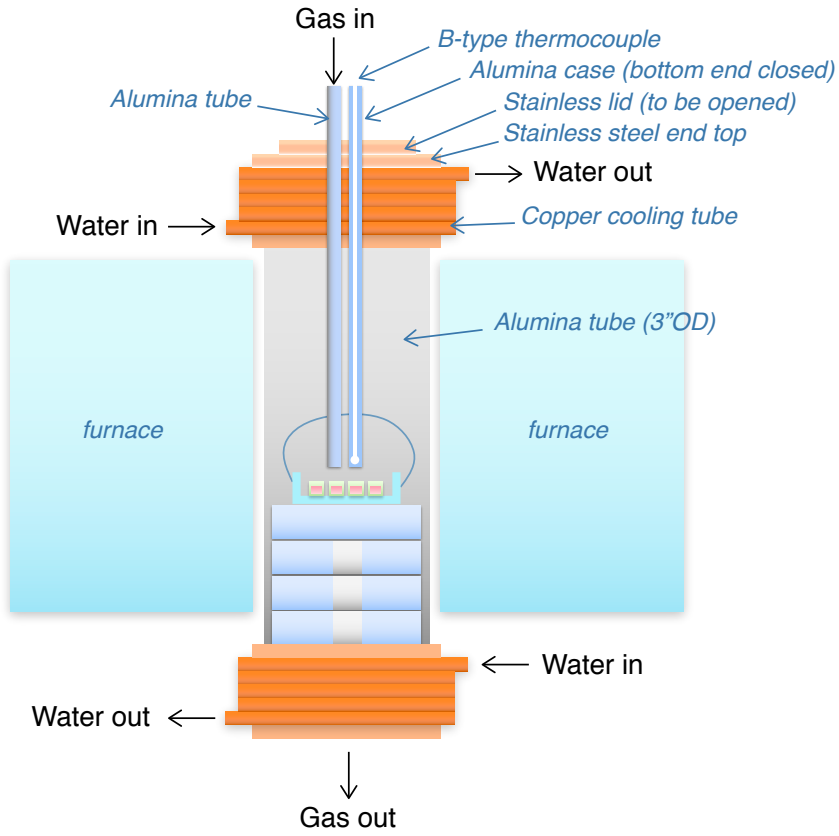

An experimental setup used to attain equilibrium in slag samples mimicking industrial compositions, placed in a simulated gasification environment.

NETL Scientists Awarded Prestigious Phase Equilibria Research Prize by the American Ceramic Society

—An NETL-RUA research team composed of scientists from NETL, URS and CMU are the recipients of the prestigious 2012 American Ceramic Society Richard and Patricia Spriggs Phase Equilibria Award. This award, given each year by the American Ceramic Society, recognizes the published work by an author, or authors, who have made a significant and lasting contribution to the fundamental understanding of phase stability relationships in ceramic-based systems. The winning research is selected from papers, articles, or reports published in a technical or trade journal, or in a bulletin from a school, laboratory, technical bureau, or experimental station, or in a pamphlet or book form.

The winning NETL-RUA team members were recognized for their article titled, "Phase Equilibria in Synthetic Coal – Petcoke Slags (Al_2O_3-CaO-FeO-SiO_2-V_2O_3) under Simulated Gasification Conditions," by Jinichiro Nakano, Kyei-Sing Kwong, James Bennett, Thomas Lam, Laura Fernandez, Piyamanee Komolwit, and Seetharaman Sridhar, and published in *Energy and Fuels 2011*, 25, 3298-3306. This research effort, which is an important piece in understanding how to optimize materials performance in fuel-flexible gasifier systems, was also recognized earlier this year by the Gustav-Eirich Award.

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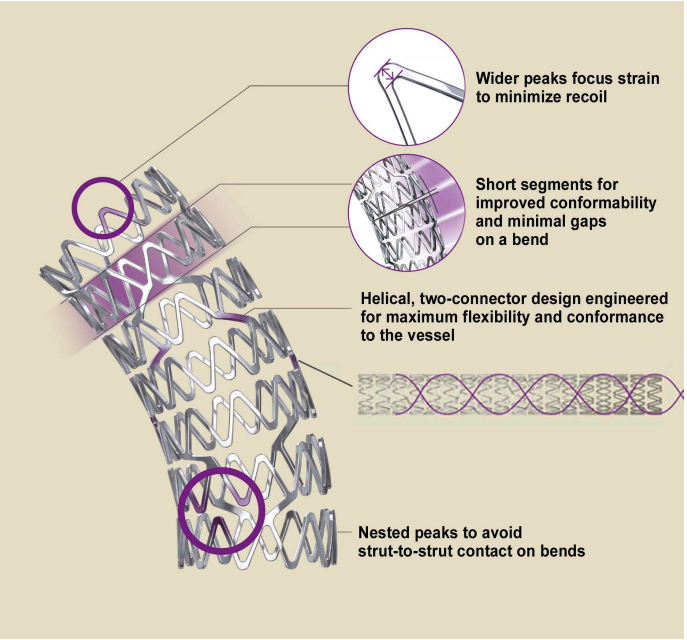

Image of platinum-chromium stent illustrating its design features. Courtesy of Boston Scientific.

Collaborative Stent Research Helps Create Hundreds of High Paying Jobs

—Heart disease is the number one cause of death in the United States and affects more than 13 million Americans. The use of coronary stents has become a mainstay of interventional cardiology, saving or improving the lives of thousands of patients each year. Stents permit the opening of blocked or restricted arteries, allowing blood to flow freely. Increased stent use required that devices with improved physical properties be developed to ensure safer and more exact placement. A crucial issue in achieving this is the ability for doctors to see the stent clearly as it is inserted through the artery to the implantation site. First- and second-generation alloys failed to achieve a balance between stent flexibility for arterial navigation and x-ray visibility for placement. To solve these problems, scientists at Boston Scientific and the U.S. Department of Energy's National Energy Technology Laboratory undertook a model industry government collaboration to develop an innovative platinum chromium (PtCr) alloy for stent manufacture The result is Boston Scientific's PtCr Stent series, which includes the PROMUS® Element™, ION™, and OMEGA™ Coronary Stent Systems.

Since ramping up production facilities in order to introduce the NETL/Boston Scientific Corporation (BSCI) platinum chromium (PtCr) alloy-based stent systems in 2010, 300 new jobs have been created at Boston Scientific alone--many in skilled, highly paying engineering and production positions. Well over 100 more are employed in the supply chain that produces these stents exclusively in the United States and ships them around the world. BSCI anticipates more job creation when the next two stents series are approved for marketing in the United States and throughout the rest of the world.

In addition, Carpenter Specialty Alloys, a major specialty steel company in Pennsylvania and the industrial producer of the PtCr alloy, was experiencing the same challenges as others manufacturers across the country during the present economic downturn. This new challenge spurred the company to invest in upgrading its research and development facility, which has since invigorated the company by delivering pilot-production quantities needed for pre-clinical and clinical studies allowing it to retain and create more jobs. The company's small-scale production line added new jobs, too.

The PtCr Element stent series is now approved for sale worldwide. It has become the global coronary stent of choice. The four PtCr coronary stent product lines have a 45% market share in the United States and a 33% worldwide market share making it the number one coronary stent in sales, which are now well in excess of $3 billion. This dramatic global adoption achieved in the series' introductory years is a tribute to its unprecedented effectiveness. These devices benefit patients by shortening recovery time and avoiding follow-on procedures and more invasive surgery. Physicians are demanding it because of ease in delivery, visibility, and improved clinical outcomes. The key to this success is the new alloy developed by NETL in collaboration with Boston Scientific that allows for a greatly improved stent design while taking advantage of all of the strengths of the PtCr alloy. This alloy was recognized in 2011 by *R&D Magazine* with an R&D 100 award.

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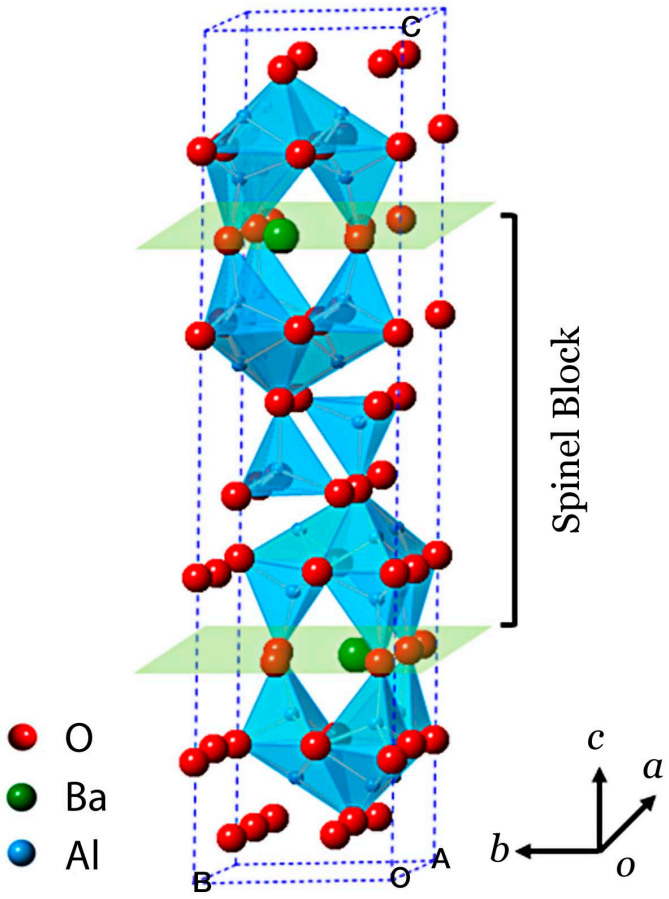

Hexaaluminate unit cell illustration.

NETL Issued Patent for Novel Catalyst Technology

—The U.S. Patent and Trademark Office recently awarded NETL U.S. Patent No. 8,142,756 for the invention of a a method to reform hydrocarbon fuels using hexaaluminate catalysts. In general, the method successfully disrupts the formation of carbon that leads to the deactivation of the catalysts, a key element in the reforming of hydrocarbon fuels. Reactions that lead to catalyst deactivation through carbon deposition and sulfur poisoning are structure sensitive and their selectivity is strongly influenced by active site dispersion and coordination. In hexaaluminate-type compounds, aluminum atoms that comprise the lattice are substitutable with catalytically active metals such as nickel. This property, when combined with its adjustable unit cell parameters, allows tailoring of surface properties that affect catalytic activity and deactivation resistance.

The patent is entitled "Methods of Reforming Hydrocarbon Fuels Using Hexaaluminate Catalysts" by Todd Gardner, Dushyant Shekhawat, and David Berry. In a series of articles (Gardner et al., J. *Phy. Chem. C* 114, 2010, 7888-7894 and Catal. Today 157, 2010, 166-169), the unique structural and catalytic properties of these materials are characterized. The technology could potentially compete with conventional methane reforming catalyst technology, and it is useful for dry reforming, partial oxidation, and steam reforming applications.

Contact: Todd Gardner, 304-285-4226

NETL Releases New Energy Analysis Tool

—Collaborators at NETL and Sandia National Laboratories have developed the Power Systems Life Cycle Analysis Tool (Power LCAT) to help policy-makers, students, and interested stakeholders better understand the economic and environmental tradeoffs associated with various electricity production options. Power LCAT is a high-level dynamic model that facilitates comparing production costs and environmental performance for several electricity generation technologies: natural gas-combined cycle, integrated gasification-combined cycle, supercritical pulverized coal, conventional pulverized coal, nuclear, and wind (with and without backup power). Fossil fuel technologies can all be configured with or without carbon capture and sequestration for analysis purposes. The model, which is based on NETL life cycle analysis reports, allows for a quick evaluation of sensitivity to key technical and financial assumptions such as construction time, heat rates, capacity factors, fuel cost, capital cost, operations and maintenance costs, interest rates, taxes, and depreciation. Power LCAT can be downloaded from the NETL Energy Analysis Models and Tools webpage.

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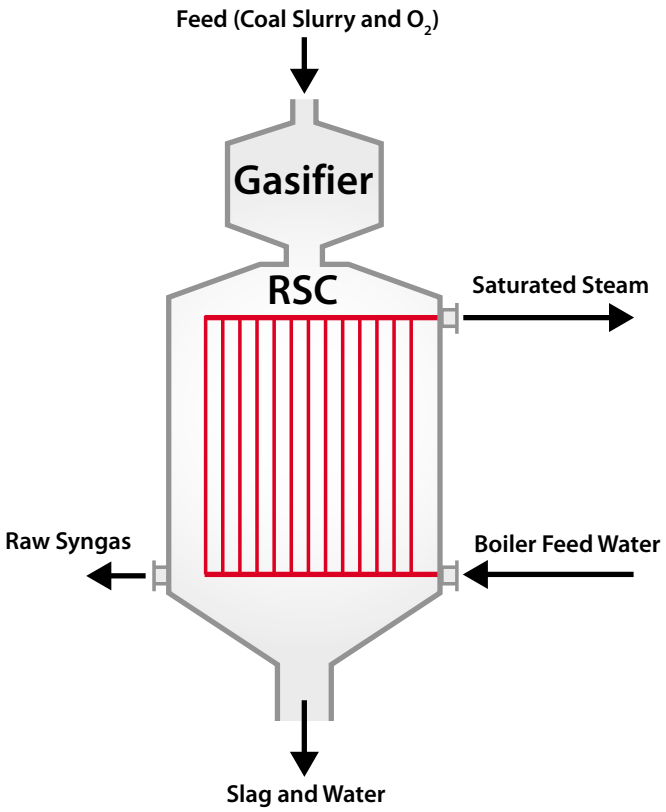


Schematic of the entrained-flow gasifier with radiant syngas cooler (RSC) considered in the study.

AVESTAR Team Improves Modeling of Entrained-Flow Gasifiers for Use in IGCC Performance Optimization Studies

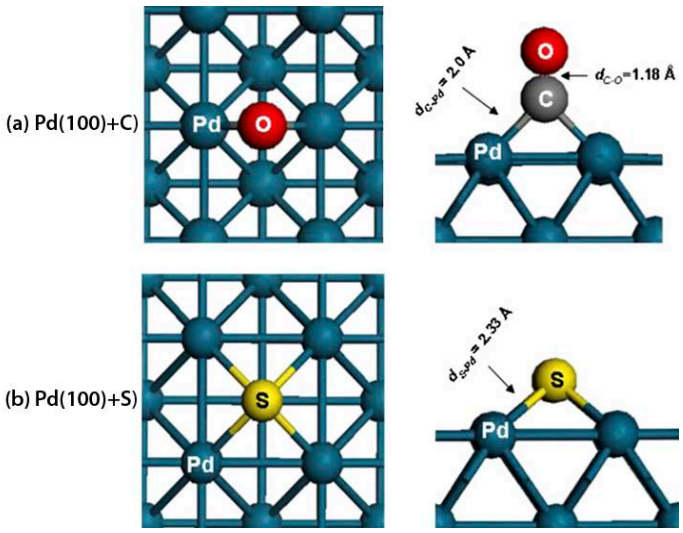
—Gasifiers are the centerpieces of fossil energy-fired IGCC power plants. To gain valuable insights into overall IGCC system performance as gasifier inlet and operating conditions change, AVESTAR researchers at NETL and West Virginia University developed a one-dimensional steady-state model of a single-stage, downward-firing, oxygen-blown, slurry-fed, entrained-flow gasifier for use in the context of IGCC process optimization. In this mathematical model, mass, momentum, and energy balance equations for solid and gas phases are considered. The model includes a number of heterogeneous and homogeneous chemical reactions along with devolatilization and drying of the slurry feed. The solid-gas heterogeneous reaction rates are calculated using the unreacted shrinking-core model.

A detailed model of the radiative heat transfer has been developed considering interactions between the solids and all internal gasifier surfaces, as well as interactions between the surfaces themselves. In the current slurry-fed gasifier model, a heuristic recirculation model has been developed to account for rapid mixing of the slurry feed with a portion of the hot reaction products which results in a significant rise in temperature that helps in evaporating the water and devolatilizing the coal.

The gasifier model is used to simulate the gasification of a wide range of different coal types. Presented as profiles for species concentration and gas, solid, and wall temperatures, the simulation results show a strong dependence of the product composition and maximum phase temperatures on the type of the coal fed to the gasifier. The optimum range for the water-to-coal and oxygen-to-coal ratios necessary for achieving at least 99 percent carbon conversion for the cases considered in the study is 0.3-0.4 and 0.8-0.9, respectively.

The gasifier model results also compare well to available pilot plant and industrial data. A paper titled "Mathematical Modeling of a Single-Stage, Downward-Firing, Entrained-Flow Gasifier," which describes these latest gasifier modeling advances, was recently published in the peer-reviewed journal, *Industrial & Engineering Chemistry Research*.

Contact: Stephen E. Zitney, 304-285-1379



Top and side view of the most stable configuration of (a) carbon monoxide (CO) and (b)sulfur (S) on palladium (Pd)(100). Gray, red, blue and yellow spheres represent C, O, Pd and S atoms, respectively.

New Study Published on Poisoning by Sulfur

—Sulfur contaminants have a highly poisonous effect on various materials used for energy applications. Uncontrollable and accidental sulfur poisoning could incur great cost to the economy. For example, metal-based membranes proposed as candidate materials for hydrogen separation are deactivated in the presence of sulfur. Much of what we know theoretically about sulfur poisoning is largely based on first-principles calculations. However, the information obtained from this method alone is not sufficient to understand sulfur poisoning-related phenomenon at finite temperature and pressure or for quantitative comparison with experiments.

Using carbon monoxide on sulfur-covered palladium as a model system, a hybrid approach was used (in which results from first-principles quantum mechanical calculations were combined with Kinetic Monte Carlo) to improve our understanding of the negative effect of sulfur on the chemical activity of palladium. The multi-scale flavor of this approach allowed the researcher to cope with intricacies that could not be modeled by the first-principles method alone.

As a result of this study, an invited paper entitled "Influence of Sulfur Poisoning on CO Adsorption on Pd(100)," authored by NETL researcher Dominic Alfonso, was published in the peer-reviewed journal *Topics in Catalysis*, titled "Influence of Sulfur Poisoning on CO adsorption on Pd(100)," *Topics in Catalysis* Vol. 55, p. 267-279 (2012).

This is the first published computational work done at NETL that uses an algorithm that can access large time and length scales (with input kinetic parameters obtained from quantum mechanical electronic structure calculations) to examine sulfur poisoning-related phenomenon. It provides a theoretical confirmation that sulfur can completely deactivate the metal at room temperature at fairly small sulfur coverage. Another key finding is that the mobility of CO is dramatically reduced by sulfur poisoning.

Contact: Dominic Alfonso, 412-386-4113

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3.	Alfonso, Dominic R., June 2012. Influence of Sulfur Poisoning on CO Adsorption on Pd(100), Topics in Catalysis, 55 (5-6) 267-279.
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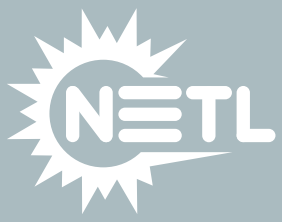
No patents issued issued this quarter



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